

Searching for Missing Binary Equiatomic Phases:

Oliyntyk, Anton O.; Gaultois, Michael W.; Hermus, Martin; Morris, Andrew; Mar, Arthur; Brgoch, Jakoah

DOI:

[10.1021/acs.inorgchem.8b01122](https://doi.org/10.1021/acs.inorgchem.8b01122)

[10.1021/acs.inorgchem.8b01122](https://doi.org/10.1021/acs.inorgchem.8b01122)

License:

None: All rights reserved

Document Version

Peer reviewed version

Citation for published version (Harvard):

Oliyntyk, AO, Gaultois, MW, Hermus, M, Morris, A, Mar, A & Brgoch, J 2018, 'Searching for Missing Binary Equiatomic Phases: Complex Crystal Chemistry in the Hf-In System', *Inorganic Chemistry*, vol. 57, no. 13, pp. 7966-7974. <https://doi.org/10.1021/acs.inorgchem.8b01122>, <https://doi.org/10.1021/acs.inorgchem.8b01122>

[Link to publication on Research at Birmingham portal](#)

Publisher Rights Statement:

Checked for eligibility: 28/06/2018

This document is the Accepted Manuscript version of a Published Work that appeared in final form in *Inorganic Chemistry*, copyright © American Chemical Society after peer review and technical editing by the publisher. To access the final edited and published work see: <https://pubs.acs.org/doi/10.1021/acs.inorgchem.8b01122>

General rights

Unless a licence is specified above, all rights (including copyright and moral rights) in this document are retained by the authors and/or the copyright holders. The express permission of the copyright holder must be obtained for any use of this material other than for purposes permitted by law.

- Users may freely distribute the URL that is used to identify this publication.
- Users may download and/or print one copy of the publication from the University of Birmingham research portal for the purpose of private study or non-commercial research.
- User may use extracts from the document in line with the concept of 'fair dealing' under the Copyright, Designs and Patents Act 1988 (?)
- Users may not further distribute the material nor use it for the purposes of commercial gain.

Where a licence is displayed above, please note the terms and conditions of the licence govern your use of this document.

When citing, please reference the published version.

Take down policy

While the University of Birmingham exercises care and attention in making items available there are rare occasions when an item has been uploaded in error or has been deemed to be commercially or otherwise sensitive.

If you believe that this is the case for this document, please contact UBIRA@lists.bham.ac.uk providing details and we will remove access to the work immediately and investigate.

SUPPORTING INFORMATION

Searching for Missing Binary Equiatomic Phases: Complex Crystal Chemistry in the Hf–In System

Anton O. Oliynyk,^{†,§,*} Michael W. Gaultois,[‡] Martin Hermus,[†] Andrew J. Morris,^{\$} Arthur Mar,^{\$} and Jakoah Brgoch[†]

[†] *Department of Chemistry, University of Houston, Houston, TX 77204 USA*

^{\$} *Department of Chemistry, University of Alberta, Edmonton, AB T6G 2G2 Canada*

[‡] *Leverhulme Research Centre for Functional Materials Design, Materials Innovation Factory, Department of Chemistry, University of Liverpool, Liverpool L7 3NY, United Kingdom*

^{\$} *School of Metallurgy and Materials, University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom*

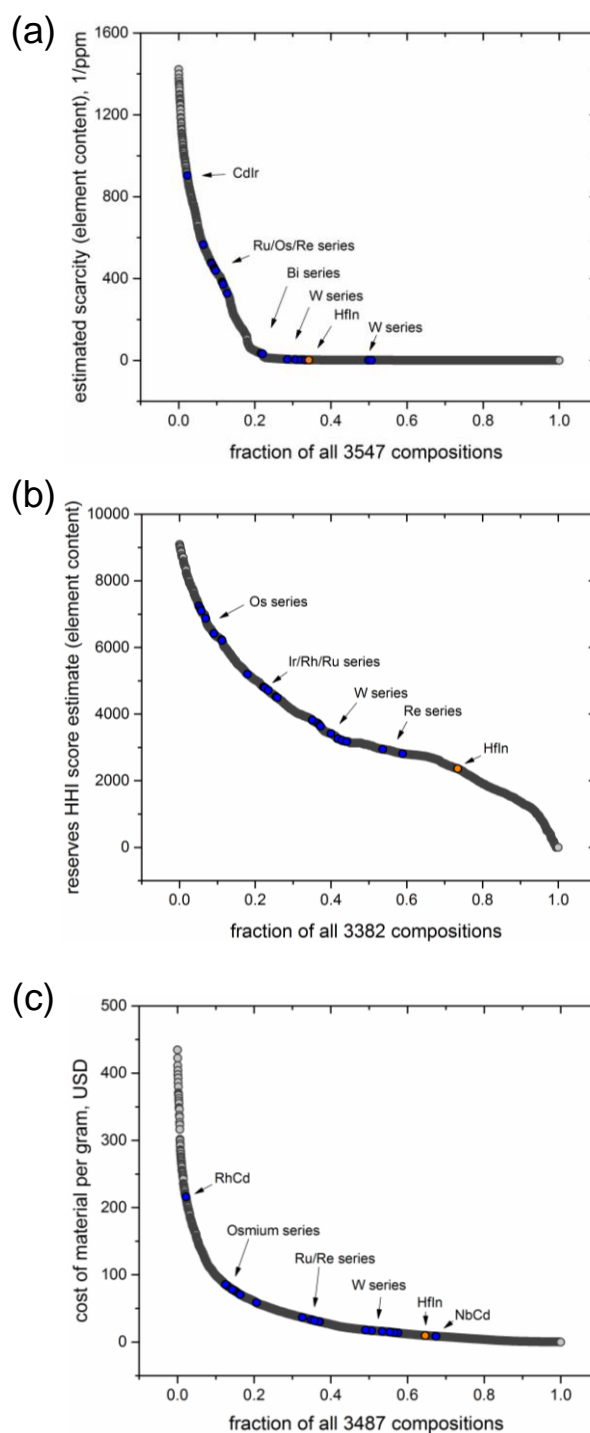


Figure S1. Estimated (a) scarcity, (b) HHI reserve score (excluding U- and Th-containing compounds), and (c) cost per gram (excluding Pm-containing compounds) for all possible AB combinations, with 21 uninvestigated systems highlighted. Calculations were made on the basis of a scarcity calculator and vendor internet prices.

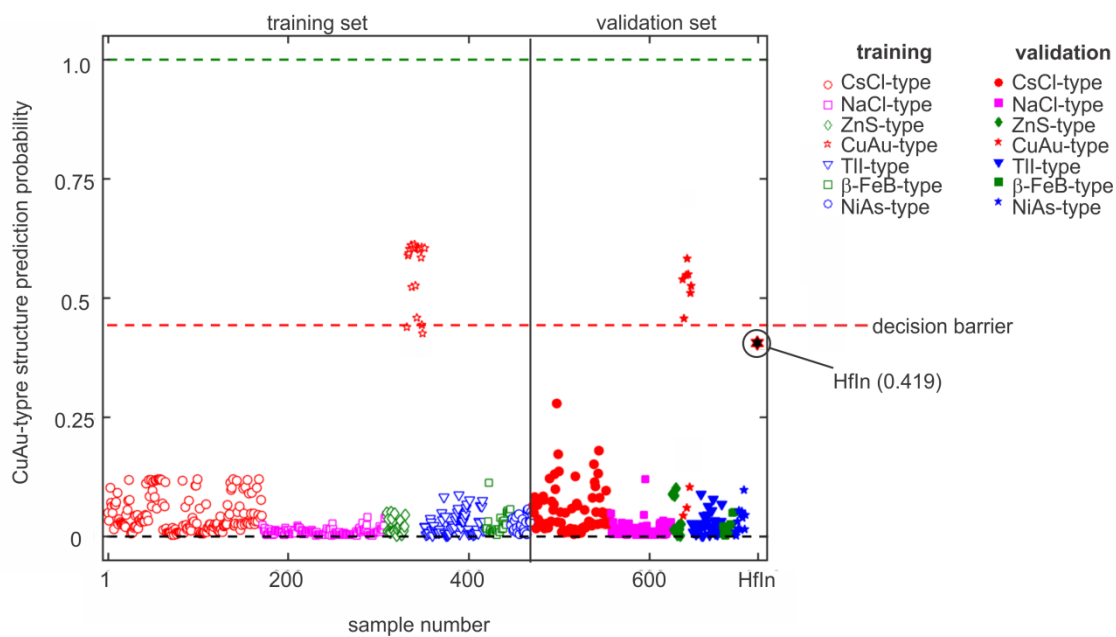
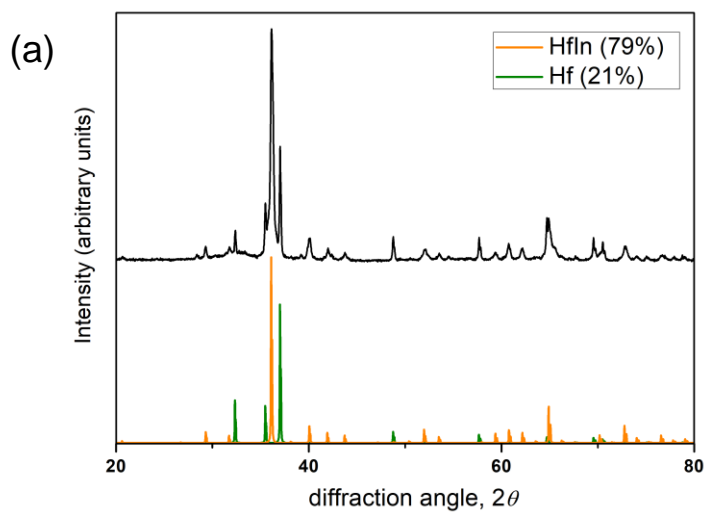


Figure S2. Probabilities predicted by machine-learning model to adopt CuAu-type structures for *AB* compounds, including HfIn.



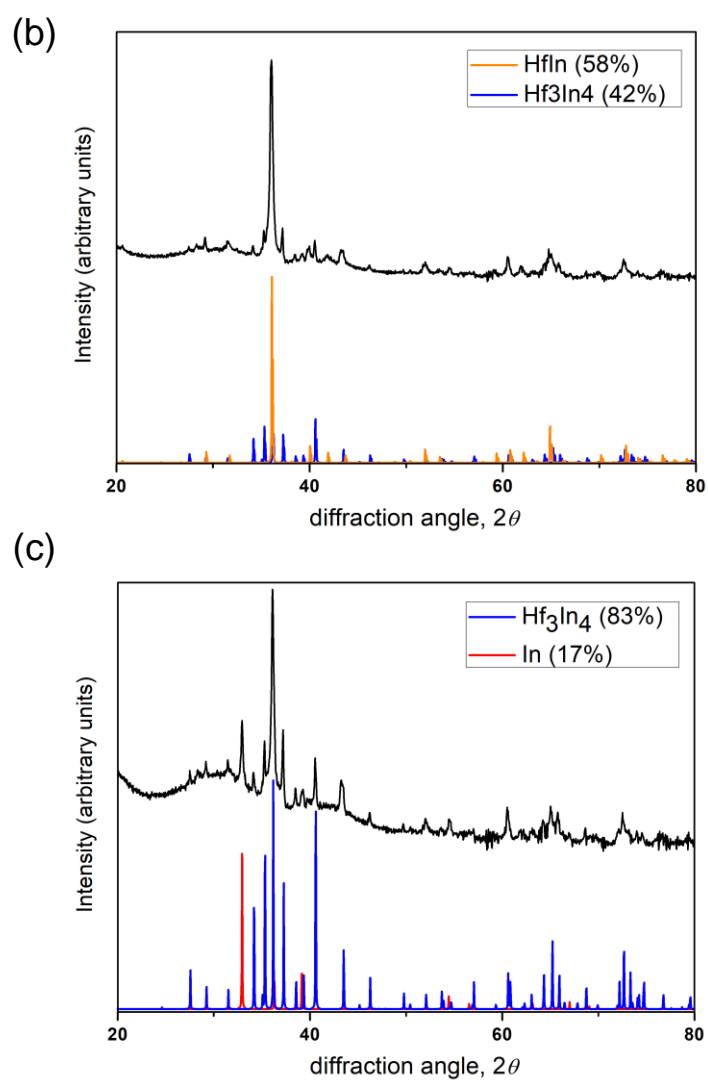


Figure S3. Powder XRD patterns for two-phase samples in Hf–In system.

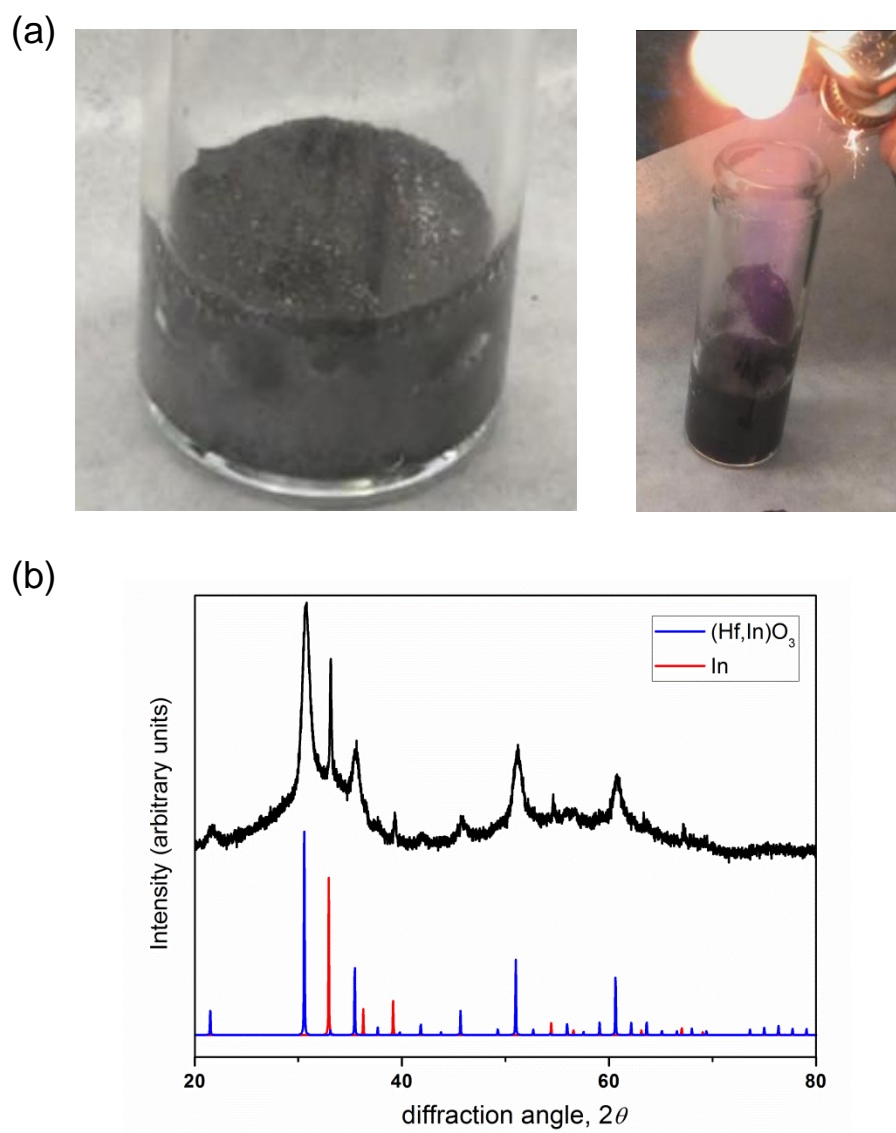


Figure S4. (a) Reaction of HfIn with water and ignition of flammable gas produced. (b) Powder XRD pattern of product after reaction with water.